Confined helium on Lagrange meshes

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Abstract

The Lagrange-mesh method has the simplicity of a calculation on a mesh and can have the accuracy of a variational method. It is applied to the study of a confined helium atom. Two types of confinement are considered. Soft confinements by potentials are studied in perimetric coordinates. Hard confinement in impenetrable spherical cavities is studied in a system of rescaled perimetric coordinates varying in [0,1] intervals. Energies and mean values of the distances between electrons and between an electron and the helium nucleus are calculated. A high accuracy of 11 to 15 significant figures is obtained with small computing times. Pressures acting on the confined atom are also computed. For sphere radii smaller than 1, their relative accuracies are better than 10^{-10}. For larger radii up to 10, they progressively decrease to 10^{-3}, still improving the best literature results.

1 Introduction

Many numerical techniques exist for quantum-mechanical calculations in configuration space. Among them, two main qualities may be searched: accuracy and simplicity. However, they are not often encountered simultaneously. For some problems, the Lagrange-mesh method has the accuracy of a variational method and the simplicity of a calculation on a mesh [1, 2, 3, 4, 5]. This approximate variational method involves a basis of Lagrange functions, i.e. infinitely differentiable functions vanishing at all mesh points of a Gauss quadrature, except one. With the help of the associated Gauss quadrature, all matrix elements are very simple. In particular, the matrix elements of the potential are approximated by values of the potential at mesh points like in collocation methods.

The striking property of the Lagrange-mesh method is that, in spite of its simplicity, it has essentially the same accuracy as a variational calculation performed with the same Lagrange basis. This performance is not well understood yet [3]. However, the accuracy of the method depends on the validity of the Gauss quadrature. Hence, the

method can be very bad in the presence of singularities of the potential. This problem can sometimes be cured by a so-called regularization [2, 3, 4, 5]. The method has been successfully applied to many problems in atomic, molecular and nuclear physics (see Ref. [5] for a review). It is particularly useful to solve coupled-channel problems in the continuum [6, 7] or three-body problems [8, 9].

The aim of the present paper is to apply the Lagrange-mesh method to a three-body problem: a helium atom confined in some environment [10, 11, 12, 13, 14, 15, 16]. The confinement can simulate a helium gas under pressure or helium atoms trapped in some molecule, carbon cluster or crystal. As we show below, existing techniques [17] are very convenient for soft confinements by potentials but can not be applied for an atom confined in an impenetrable spherical cavity. The difficulty arises from simultaneously meeting two different constraints: regularizing the singularities of the three Coulomb terms and forcing the confinement. The former condition is easily treated in perimetric coordinates [18, 19] which automatically regularize the singularities but which necessarily extend over the whole configuration space. Confinement is easily and accurately treated on a Lagrange mesh over a finite interval for hydrogen [20, 5]. Here we show that a new coordinate system can be built for helium which keeps the regularization of the potential but over an impenetrable spherical cavity.

The principle of the Lagrange-mesh method is recalled in section 2. In section 3, the problem of the confined helium atom is presented. In section 4, the Lagrange-mesh method in perimetric coordinates is recalled. A new system of coordinates is introduced in section 5 as well as its Lagrange-mesh implementation. Results for the different types of confinement are discussed on section 6. Concluding remarks are presented in section 7.

2 Principle of the Lagrange-mesh method

Let us consider N mesh points x_i associated with a Gauss-quadrature approximation [21],

$$\int_0^\infty F(x)dx \approx \sum_{k=1}^{N} \lambda_k F(x_k). \tag{1}$$

The weight coefficients λ_i are also called Christoffel numbers. Lagrange functions are a set of N orthonormal functions $f_j(x)$ associated with this mesh verifying two conditions [1, 4, 5]. (i) They satisfy the Lagrange property

$$f_j(x_i) = \lambda_i^{-1/2}\delta_{ij}, \tag{2}$$

i.e., they vanish at all mesh points, but one. (ii) The Gauss quadrature is exact for products of two Lagrange functions.

Let us consider a particle of mass m in a potential $V(x)$. This basis is used in an approximate variational calculation with the trial function

$$\psi(x) = \sum_{j=1}^{N} c_j f_j(x). \tag{3}$$

The matrix elements of potential $V(x)$ are calculated at the Gauss approximation as

$$\langle f_i|V|f_j\rangle \approx \sum_{k=1}^{N} \lambda_k f_i(x_k) V(x_k) f_j(x_k) = V(x_i)\delta_{ij} \tag{4}$$

because of the Lagrange property (2). The variational equations then take the form of mesh equations [1, 4, 5]

$$\sum_{j=1}^{N} \left(\frac{\hbar^2}{2m} T_{ij} + V(x_i)\delta_{ij} \right) c_j = E c_i, \tag{5}$$

where the exact or approximate matrix elements $T_{ij} = \langle f_i| - d^2/dx^2|f_j\rangle$ have simple known expressions as a function of the zeros x_i and x_j. See Refs. [1, 4, 5] for details.

This simple approximation can be very accurate with small numbers of mesh points when the Gauss approximation is valid for the potential matrix elements, i.e. when the potential and its derivatives have no singularities. In the presence of singularities, the basis can sometimes be regularized by multiplying the Lagrange functions by a convenient factor $R(x)$ [2, 4, 5],

$$\hat{f}_j(x) = \frac{R(x)}{R(x_j)} f_j(x). \tag{6}$$

The regularized functions $\hat{f}_j(x)$ still verify the Lagrange conditions (2) but they are not orthogonal anymore, in general. However, they are still orthogonal at the Gauss-quadrature approximation and can still be treated as orthonormal in the Lagrange-mesh method without significant loss of accuracy [3, 5]. Such a regularization is also useful when the particle is confined by an impenetrable wall [20] (see section 5).

3 Confined helium

We consider a two-electron atom with an infinite-mass nucleus of charge Ze. This nucleus is fixed and the electrons are characterized by coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ with respect to this nucleus. In atomic units $\hbar = m_e = a_0 = e = 1$, where m_e is the electron mass and a_0 is the Bohr radius, the Hamiltonian of the helium atom reads

$$H = T + V_C = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \tag{7}$$

where

$$\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2 \tag{8}$$

and Δ_1 and Δ_2 are the Laplacians with respect to $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$.

For a free atom, the wave functions of the bound states must vanish at infinity. A confinement can be introduced in the problem either by forcing the wave function into some spherical cavity (hard confinement) or by adding a confining potential to H (soft confinement).

Hard confinement is obtained with the conditions

$$r_1 \leq R, \quad r_2 \leq R. \tag{9}$$

The wave function $\psi(r_1, r_2, r_{12})$ of an S state must thus verify

$$\psi(R, r_2, r_{12}) = \psi(r_1, R, r_{12}) = 0. \tag{10}$$

Soft confinement can be obtained by adding a potential $V_{\rm conf}(r_1, r_2)$ which tends to a large positive constant or to infinity when r_1 or r_2 tends to infinity. The role of this potential is to reduce the probability density of presence of the electrons at large distances.

Let us start with the soft confinement since it can be treated with the same code as for the free atom with only a tiny modification [17].

4 Lagrange mesh for soft confinement

4.1 Perimetric coordinates

The system of perimetric coordinates [18, 19] is very convenient for Lagrange-mesh calculations of three-body systems because the three dimensioned coordinates are independent from each other and vary from zero to infinity. Moreover, the volume element automatically regularizes the singularities of the three Coulomb potentials [17].

The perimetric coordinates are composed of three Euler angles and the three coordinates

$$\begin{aligned} x &= r_1 - r_2 + r_{12}, \\ y &= -r_1 + r_2 + r_{12}, \\ z &= r_1 + r_2 - r_{12}. \end{aligned} \tag{11}$$

The volume element of the dimensioned coordinates reads

$$dV = (x+y)(y+z)(z+x)dxdydz. \tag{12}$$

In perimetric coordinates, the Coulomb potentials become

$$V_C(x, y, z) = -\frac{2Z}{z+x} - \frac{2Z}{y+z} + \frac{2}{x+y}. \tag{13}$$

With the volume element dV, the integrand in matrix elements of this potential is bounded everywhere. Hence the Gauss quadrature and the Lagrange-mesh method are accurate.

The kinetic-energy operator T is rather complicated [22]. It is convenient to write its matrix elements in a symmetric form [23, 17],

$$\langle F|T|G\rangle = 2\int_0^\infty dx \int_0^\infty dy \int_0^\infty dz \sum_{i,j=1}^{3} A_{ij}(x, y, z) \frac{\partial F}{\partial x_i} \frac{\partial G}{\partial x_j}, \tag{14}$$

where $(x_1, x_2, x_3) \equiv (x, y, z)$. The coefficients A_{ij} are given by

$$\begin{aligned} A_{11} &= x(y+z)(x+y+z) + xz(z+x), \\ A_{22} &= yz(y+z) + y(z+x)(x+y+z), \\ A_{33} &= yz(y+z) + xz(z+x), \\ A_{12} &= A_{21} = 0, \\ A_{13} &= A_{31} = -xz(z+x), \\ A_{23} &= A_{32} = -yz(y+z). \end{aligned} \tag{15}$$

4.2 Lagrange mesh and functions

The Lagrange-Laguerre functions are defined as [1]

$$f_j(x) = (-1)^j x_j^{1/2} \, \frac{L_N(x)}{x - x_j} \, e^{-x/2}, \tag{16}$$

where $L_N(x)$ is the Laguerre polynomial of degree N and the x_i are its zeros,

$$L_N(x_i) = 0. \tag{17}$$

Notice that the Lagrange functions are linearly independent polynomials of degree $N-1$ multiplied by an exponential which is the square root of the Laguerre weight function $\exp(-x)$. The basis is thus equivalent, for example, to a basis formed of the Laguerre polynomials of degrees 0 to $N-1$ multiplied by $\exp(-x/2)$.

The functions $f_j(x)$ are associated with the Gauss-Laguerre quadrature [21]. They verify the Lagrange conditions (2) and integrals of products of two Lagrange functions are exactly given by the Gauss quadrature since the integrand is the product of the Laguerre weight function $\exp(-x)$ by a polynomial of degree $2N-2$ [24]. Functions (16) are exactly orthonormal over $(0, \infty)$.

The first derivative of a one-dimensional Lagrange-Laguerre function at mesh points is given by

$$\lambda_i^{1/2} f_j'(x_i) = (-1)^{i-j} \sqrt{\frac{x_j}{x_i}} \, \frac{1}{x_i - x_j} \tag{18}$$

for $i \neq j$ and by

$$\lambda_i^{1/2} f_i'(x_i) = -\frac{1}{2x_i}. \tag{19}$$

Three-dimensional mesh and basis are obtained as follows. Let x_p $(p = 1, \ldots, N_x)$, y_q $(q = 1, \ldots, N_y)$ and z_r $(r = 1, \ldots, N_z)$ be the zeros of Laguerre polynomials with respective degrees N_x, N_y and N_z. Three-dimensional Lagrange functions $F_{ijk}(x, y, z)$ associated with the mesh $(h_x x_p, h_y y_q, h_z z_r)$ are defined by

$$F_{ijk}(x, y, z) = \mathcal{N}_{ijk}^{-1/2} f_i^{(N_x)}(x/h_x) f_j^{(N_y)}(y/h_y) f_k^{(N_z)}(z/h_z). \tag{20}$$

The functions $f_i^{(N)}$ are given by expression (16) with N replaced by N_x, N_y or N_z. The corresponding Christoffel numbers are denoted as λ_i, μ_j and ν_k. Scale parameters h_x, h_y and h_z are introduced in order to fit the different meshes to the size of the actual physical problem. The normalization factor $\mathcal{N}_{ijk}$ is defined as

$$\mathcal{N}_{ijk} = h_x h_y h_z (h_x x_i + h_y y_j)(h_x x_i + h_z z_k)(h_y y_j + h_z z_k). \tag{21}$$

The Lagrange functions $F_{ijk}(x, y, z)$ satisfy the Lagrange property

$$F_{ijk}(h_x x_p, h_y y_q, h_z z_r) = (\mathcal{N}_{ijk} \lambda_i \mu_j \nu_k)^{-1/2} \delta_{ip} \delta_{jq} \delta_{kr}, \tag{22}$$

i.e., they vanish at all points of the three-dimensional mesh, but one. With the volume element (12), they are not orthogonal but the scalar product $\langle F_{i'j'k'} | F_{ijk} \rangle$ is calculated

with the Gauss-quadrature approximation as $\delta_{ii'}\delta_{jj'}\delta_{kk'}$. They are thus treated as an orthonormal basis in the method.

The kinetic-energy matrix elements are given by

$$\begin{aligned}
&\langle F_{i'j'k'}|T|F_{ijk}\rangle \approx 2\mathcal{N}_{i'j'k'}^{-1/2}\mathcal{N}_{ijk}^{-1/2}h_xh_yh_z \\
&\times\Big\{\delta_{jj'}\delta_{kk'}\sum_n A_{11}(h_xx_n,h_yy_j,h_zz_k)\lambda_n f_i^{(N_x)\prime}(x_n)f_{i'}^{(N_x)\prime}(x_n)h_x^{-2} \\
&+\delta_{ii'}\delta_{kk'}\sum_n A_{22}(h_xx_i,h_yy_n,h_zz_k)\mu_n f_j^{(N_y)\prime}(y_n)f_{j'}^{(N_y)\prime}(y_n)h_y^{-2} \\
&+\delta_{ii'}\delta_{jj'}\sum_n A_{33}(h_xx_i,h_yy_j,h_zz_n)\nu_n f_k^{(N_z)\prime}(z_n)f_{k'}^{(N_z)\prime}(z_n)h_z^{-2} \\
&+\delta_{kk'}\Big[A_{12}(h_xx_i,h_yy_{j'},h_zz_k)(\lambda_i\mu_{j'})^{1/2}f_{i'}^{(N_x)\prime}(x_i)f_j^{(N_y)\prime}(y_{j'}) \\
&+A_{12}(h_xx_{i'},h_yy_j,h_zz_k)(\lambda_{i'}\mu_j)^{1/2}f_i^{(N_x)\prime}(x_{i'})f_{j'}^{(N_y)\prime}(y_j)\Big](h_xh_y)^{-1} \\
&+\delta_{jj'}\Big[A_{13}(h_xx_i,h_yy_j,h_zz_{k'})(\lambda_i\nu_{k'})^{1/2}f_{i'}^{(N_x)\prime}(x_i)f_k^{(N_z)\prime}(z_{k'}) \\
&+A_{13}(h_xx_{i'},h_yy_j,h_zz_k)(\lambda_{i'}\nu_k)^{1/2}f_i^{(N_x)\prime}(x_{i'})f_{k'}^{(N_z)\prime}(z_k)\Big](h_xh_z)^{-1} \\
&+\delta_{ii'}\Big[A_{23}(h_xx_i,h_yy_j,h_zz_{k'})(\mu_j\nu_{k'})^{1/2}f_{j'}^{(N_y)\prime}(y_j)f_k^{(N_z)\prime}(z_{k'}) \\
&+A_{23}(h_xx_i,h_yy_{j'},h_zz_k)(\mu_{j'}\nu_k)^{1/2}f_j^{(N_y)\prime}(y_{j'})f_{k'}^{(N_z)\prime}(z_k)\Big](h_yh_z)^{-1}\Big\}. \qquad (23)
\end{aligned}$$

From now on, we consider $N_x = N_y = N$ which implies $x_i \equiv y_i$, $\lambda_i \equiv \mu_i$, and $h_x = h_y = h$.

The Lagrange functions are used as a variational basis to expand an S-wave trial function,

$$\psi(x,y,z) = \sum_{i=1}^{N}\sum_{j=1}^{i-\sigma}\sum_{k=1}^{N_z} C_{ijk}[2(1+\delta_{ij})]^{-1/2}[F_{ijk}(x,y,z) \pm F_{jik}(x,y,z)], \qquad (24)$$

where $\sigma = 0$ in the symmetric case and 1 in the antisymmetric case, and $j \le i - \sigma$ because of the symmetry with respect to the exchange of electrons 1 and 2. The matrix representing the total potential $V = V_C + V_{\rm conf}$ is immediately obtained with a triple Gauss quadrature and the Lagrange property (22) as

$$\langle F_{i'j'k'}|V|F_{ijk}\rangle \approx V(hx_i,hx_j,h_zz_k)\delta_{ii'}\delta_{jj'}\delta_{kk'}. \qquad (25)$$

The variational calculation then reduces to mesh-like equations

$$\begin{aligned}
\sum_{i=1}^{N}\sum_{j=1}^{i-\sigma}\sum_{k=1}^{N_z}\{&(1+\delta_{ij})^{-1/2}(1+\delta_{i'j'})^{-1/2}[\langle F_{i'j'k'}|T|F_{ijk}\rangle \pm \langle F_{i'j'k'}|T|F_{jik}\rangle] \\
&+[V(hx_i,hx_j,h_zz_k) - E]\delta_{ii'}\delta_{jj'}\delta_{kk'}\}C_{ijk} = 0. \qquad (26)
\end{aligned}$$

Energies and wave functions are obtained from the eigenvalues and eigenvectors of a large sparse symmetric matrix.

Mean values of a multiplicative operator $O(x,y,z)$ are simply given at the Gauss approximation by

$$\langle\psi|O(x,y,z)|\psi\rangle \approx \tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{i-\sigma}\sum_{k=1}^{N_z} C_{ijk}^2[O(hx_i,hx_j,h_zz_k) + O(hx_j,hx_i,h_zz_k)]. \qquad (27)$$

5 Lagrange mesh for hard confinement

5.1 Rescaled perimetric coordinates

In an impenetrable spherical cavity of radius R, the perimetric coordinates are constrained by

$$\begin{aligned} 0 \le x \le 2R - z, \\ 0 \le y \le 2R - z, \\ 0 \le z \le 2R. \end{aligned} \tag{28}$$

Hence the kinetic matrix elements (14) must be rewritten as

$$\langle F|T|G\rangle = 2\int_0^{2R} dz \int_0^{2R-z} dx \int_0^{2R-z} dy \sum_{i,j=1}^{3} A_{ij}(x,y,z) \frac{\partial F}{\partial x_i}\frac{\partial G}{\partial x_j}. \tag{29}$$

The z dependence of the upper bounds of the x and y coordinates is a difficulty for the use of the Lagrange-mesh method.

We thus introduce a new set of coordinates $(u, v, w) \equiv (u_1, u_2, u_3)$ defined over $[0, 1]$ by

$$\begin{aligned} u &= \frac{x}{2R - z}, \\ v &= \frac{y}{2R - z}, \\ w &= \frac{z}{2R}. \end{aligned} \tag{30}$$

Their upper values are indeed

$$\begin{aligned} u = 1 \quad (r_1 = R), \\ v = 1 \quad (r_2 = R), \\ w = 1 \quad (r_1 = r_2 = R, r_{12} = 0). \end{aligned} \tag{31}$$

Inversely, one has

$$\begin{aligned} x &= 2Ru(1 - w), \\ y &= 2Rv(1 - w), \\ z &= 2Rw. \end{aligned} \tag{32}$$

The volume element then becomes

$$dV = (2R)^6(u + v)(u + w - uw)(v + w - vw)(1 - w)^3 du dv dw. \tag{33}$$

The Coulomb potential reads

$$V_C(u, v, w) = \frac{1}{R}\left[-\frac{Z}{u + w - uw} - \frac{Z}{v + w - vw} + \frac{1}{(u + v)(1 - w)}\right]. \tag{34}$$

The integrands in its matrix elements are automatically regularized by the volume element. The kinetic matrix elements become

$$\langle F|T|G\rangle = 2(2R)^4 \int_0^1 du \int_0^1 dv \int_0^1 dw \sum_{i,j=1}^{3} B_{ij}(u,v,w) \frac{\partial F}{\partial u_i} \frac{\partial G}{\partial u_j} \tag{35}$$

where

$$\begin{aligned}
B_{11} &= u(1-w)\left[a_v b + (1-u)^2 w a_u\right], \\
B_{22} &= v(1-w)\left[(1-v)^2 w a_v + a_u b\right], \\
B_{33} &= w(1-w)^3\left[v a_v + u a_u\right], \\
B_{12} &= B_{21} = uvw(1-w)\left[(v-1)a_v + (u-1)a_u\right], \\
B_{13} &= B_{31} = uw(1-w)^2\left[v a_v + (u-1)a_u\right], \\
B_{23} &= B_{32} = vw(1-w)^2\left[(v-1)a_v + u a_u\right]
\end{aligned} \tag{36}$$

with

$$\begin{aligned}
a_u &= u + w - uw, \\
a_v &= v + w - vw, \\
b &= u + v + w - uw - vw + uvw.
\end{aligned} \tag{37}$$

5.2 Lagrange mesh and functions

Let us introduce a convenient basis over the $[0,1]$ interval. Regularized Lagrange-Legendre functions are defined by

$$f_j(u) = (-1)^{N-j} \sqrt{\frac{u_j}{1-u_j}} \frac{P_N(2u-1)}{u-u_j}(1-u), \tag{38}$$

where the mesh points u_i are the zeros of the shifted Legendre polynomial of degree N,

$$P_N(2u_i - 1) = 0. \tag{39}$$

They are associated with the Gauss-Legendre quadrature on the $[0,1]$ interval. The regularized Lagrange functions (38) correspond to standard Lagrange-Legendre functions [1], shifted [25] and multiplied by the factor $(1-u)/(1-u_j)$, so that they vanish at $u=1$. In Ref. [25] on the contrary, they are multiplied by u/u_j so that they vanish at $u=0$. In Ref. [20], they are multiplied by both factors simultaneously and vanish at $u=0$ and 1. Notice that all these types of regularized functions satisfy the Lagrange conditions (2) but are not orthogonal. Nevertheless they can be treated as orthonormal in Lagrange-mesh calculations without significant loss of accuracy [3, 5].

The first derivative of a Lagrange-Legendre function (38) at mesh points is given by

$$\lambda_i^{1/2} f_j'(u_i) = (-1)^{i+j} \sqrt{\frac{u_j(1-u_i)}{u_i(1-u_j)}} \frac{1}{u_i - u_j} \tag{40}$$

for $i \neq j$ and by

$$\lambda_i^{1/2} f_i'(u_i) = -\frac{1}{2u_i(1-u_i)}. \tag{41}$$

Over a three-dimensional mesh (u_p, v_q, w_r), where u_p, v_q, w_r are solutions of Eq. (39) with possibly different values N_u, N_v, N_w of N, three-dimensional Lagrange functions $F_{ijk}(u,v,w)$ are defined by

$$F_{ijk}(u,v,w) = \mathcal{N}_{ijk}^{-1/2} f_i^{(N_u)}(u) f_j^{(N_v)}(v) f_k^{(N_w)}(w) \tag{42}$$

with

$$\mathcal{N}_{ijk} = (2R)^6 (u_i + v_j)(u_i + w_k - u_i w_k)(v_j + w_k - v_j w_k)(1-w_k)^3. \tag{43}$$

These functions satisfy the Lagrange conditions

$$F_{ijk}(u_p, v_q, w_r) = (\mathcal{N}_{ijk} \lambda_i \mu_j \nu_k)^{-1/2} \delta_{ip} \delta_{jq} \delta_{kr}, \tag{44}$$

where λ_i, μ_j and ν_k are now the weights of the Gauss-Legendre quadrature over the $[0,1]$ interval with N_u, N_v and N_w points, respectively. They are not orthogonal but they are orthonormal at the Gauss-quadrature approximation and are treated as an orthonormal basis in the method,

$$\langle F_{i'j'k'} | F_{ijk} \rangle \;\rightarrow\; \delta_{ii'} \delta_{jj'} \delta_{kk'}. \tag{45}$$

The kinetic matrix elements are given by

$$\begin{aligned}
&\langle F_{i'j'k'} | T | F_{ijk} \rangle \approx 2(2R)^4 \mathcal{N}_{i'j'k'}^{-1/2} \mathcal{N}_{ijk}^{-1/2} \\
&\times \Big\{ \delta_{jj'} \delta_{kk'} \sum_n B_{11}(u_n, v_j, w_k) \lambda_n f_i^{(N_u)\prime}(u_n) f_{i'}^{(N_u)\prime}(u_n) \\
&+ \delta_{ii'} \delta_{kk'} \sum_n B_{22}(u_i, v_n, w_k) \mu_n f_j^{(N_v)\prime}(v_n) f_{j'}^{(N_v)\prime}(v_n) \\
&+ \delta_{ii'} \delta_{jj'} \sum_n B_{33}(u_i, v_j, w_n) \nu_n f_k^{(N_w)\prime}(w_n) f_{k'}^{(N_w)\prime}(w_n) \\
&+ \delta_{kk'} \Big[B_{12}(u_i, v_{j'}, w_k) (\lambda_i \mu_{j'})^{1/2} f_{i'}^{(N_u)\prime}(u_i) f_j^{(N_v)\prime}(v_{j'}) \\
&+ B_{12}(u_{i'}, v_j, w_k) (\lambda_{i'} \mu_j)^{1/2} f_i^{(N_u)\prime}(u_{i'}) f_{j'}^{(N_v)\prime}(v_j) \Big] \\
&+ \delta_{jj'} \Big[B_{13}(u_i, v_j, w_{k'}) (\lambda_i \nu_{k'})^{1/2} f_{i'}^{(N_u)\prime}(u_i) f_k^{(N_w)\prime}(w_{k'}) \\
&+ B_{13}(u_{i'}, v_j, w_k) (\lambda_{i'} \nu_k)^{1/2} f_i^{(N_u)\prime}(u_{i'}) f_{k'}^{(N_w)\prime}(w_k) \Big] \\
&+ \delta_{ii'} \Big[B_{23}(u_i, v_j, w_{k'}) (\mu_j \nu_{k'})^{1/2} f_{j'}^{(N_v)\prime}(v_j) f_k^{(N_w)\prime}(w_{k'}) \\
&+ B_{23}(u_i, v_{j'}, w_k) (\mu_{j'} \nu_k)^{1/2} f_j^{(N_v)\prime}(v_{j'}) f_{k'}^{(N_w)\prime}(w_k) \Big] \Big\}.
\end{aligned} \tag{46}$$

From now on, we take $N_u = N_v = N$.

An S-wave trial function is expanded as

$$\psi(u,v,w) = \sum_{i=1}^{N} \sum_{j=1}^{i-\sigma} \sum_{k=1}^{N_w} C_{ijk} [2(1+\delta_{ij})]^{-1/2} [F_{ijk}(u,v,w) \pm F_{jik}(u,v,w)], \tag{47}$$

where σ is defined as above. The potential matrix elements simply read

$$\langle F_{i'j'k'}|V_C|F_{ijk}\rangle \approx \delta_{ii'}\delta_{jj'}\delta_{kk'} \times\frac{1}{R}\left[-\frac{Z}{u_i+w_k-u_iw_k}-\frac{Z}{u_j+w_k-u_jw_k}+\frac{1}{(u_i+u_j)(1-w_k)}\right]. \quad (48)$$

The Lagrange-mesh equations are

$$\sum_{i=1}^{N}\sum_{j=1}^{i-\sigma}\sum_{k=1}^{N_w}\{(1+\delta_{ij})^{-1/2}(1+\delta_{i'j'})^{-1/2}[\langle F_{i'j'k'}|T|F_{ijk}\rangle \pm \langle F_{i'j'k'}|T|F_{jik}\rangle] +[V_C(u_i,u_j,w_k)-E]\delta_{ii'}\delta_{jj'}\delta_{kk'}\}C_{ijk}=0. \quad (49)$$

Notice that obtaining energies does not require calculating eigenvalues of a generalized eigenvalue problem since the basis is treated as orthonormal.

Mean values of a multiplicative operator $O(u,v,w)$ are given at the Gauss approximation by

$$\langle\psi|O(u,v,w)|\psi\rangle \approx \tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{i-\sigma}\sum_{k=1}^{N_w}C_{ijk}^2[O(u_i,u_j,w_k)+O(u_j,u_i,w_k)]. \quad (50)$$

6 Results

All results are presented in atomic units except in Table 7. An error of a few units may affect the last displayed digit.

6.1 Soft confinement

The study of soft confinement is performed in perimetric coordinates using the code of Ref. [17] with two modifications. (i) A confining potential $V_{\rm conf}$ is added to the Coulomb potential; this is a very simple addition in the code since no matrix elements are needed. (ii) The search of the lowest eigenvalues of the rather scarce Hamiltonian matrix is now performed with the Jacobi-Davidson algorithm [26]. Mean values are calculated with Eq. (27) for the distance r_{12} between electrons and for the distances r_1 and r_2 between the electrons and the nucleus.

The calculations are performed to provide 12-15 significant figures in the fastest way, when such an accuracy can be reached with reasonable basis sizes. The calculation starts with a search for an optimal domain of the scale parameters h and h_z. The significant digits are obtained by comparison between several calculations with different numbers of mesh points. The simplest of the calculations giving the requested accuracy is then kept.

As a first penetrable confinement, we choose like in Ref. [12] the harmonic potential

$$V_{\rm conf}(r_1,r_2)=\tfrac{1}{2}\omega^2(r_1^2+r_2^2), \quad (51)$$

where ω is a parameter. The convergence for $\omega=1$ is studied in Table 1 as a function of the numbers N and N_z. The total mesh size $N_T=\frac{1}{2}N(N+1)N_z$ is also given.

The parameters h and h_z are roughly optimized. One observes a fast convergence for $h=0.15-0.20$ and $h_z=0.15-0.20$ where very accurate results are already obtained

Table 1: Convergence of the ground-state energy and the mean interparticle distances of a helium atom confined by the harmonic potential (51) with $\omega = 1$ as a function of the numbers N and N_z of mesh points and the total mesh size N_T.

N	N_z	N_T	h	h_z	E	$\langle r_{12} \rangle$	$\langle r_1 \rangle = \langle r_2 \rangle$
10	10	550	0.15	0.20	−2.073 075 9	1.085 817 9	0.723 715 2
			0.20	0.20	−2.073 035 387 6	1.085 686 267 07	0.723 644 406 9
15	15	1800	0.15	0.20	−2.073 035 362 032 5	1.085 685 768 807 16	0.723 644 141 796 32
			0.20	0.20	−2.073 035 362 047 7	1.085 685 768 608 92	0.723 644 141 692 94
20	20	4200	0.15	0.20	−2.073 035 362 051 89	1.085 685 768 624 21	0.723 644 141 700 93
			0.20	0.20	−2.073 035 362 051 54	1.085 685 768 624 56	0.723 644 141 701 14
25	20	6500	0.15	0.20	−2.073 035 362 051 95	1.085 685 768 624 25	0.723 644 141 700 96
			0.20	0.20	−2.073 035 362 051 88	1.085 685 768 624 25	0.723 644 141 700 96
25	25	8125	0.15	0.20	−2.073 035 362 051 94	1.085 685 768 624 19	0.723 644 141 700 92
			0.20	0.20	−2.073 035 362 051 86	1.085 685 768 623 99	0.723 644 141 700 80
30	25	11625	0.15	0.20	−2.073 035 362 051 94	1.085 685 768 624 13	0.723 644 141 700 88
			0.20	0.20	−2.073 035 362 051 94	1.085 685 768 624 22	0.723 644 141 700 93
30	30	13950	0.15	0.20	−2.073 035 362 051 93	1.085 685 768 624 21	0.723 644 141 700 91
			0.20	0.20	−2.073 035 362 051 91	1.085 685 768 624 23	0.723 644 141 700 93
Ref. [12]					−2.073 035		

Table 2: Ground-state energy and mean interparticle distances of a helium atom confined by the harmonic potential (51) as a function of the numbers N and N_z of mesh points and the scale parameters h and h_z.

ω	N	N_z	h	h_z	E	$\langle r_{12} \rangle$	$\langle r_1 \rangle = \langle r_2 \rangle$
0	30	25	0.30	0.35	−2.903 724 377 034 0	1.422 070 255 565 9	0.929 472 294 873 7
0.01	30	25	0.30	0.35	−2.903 605 041 422 9	1.421 940 016 512 7	0.929 395 600 292 0
0.05	30	25	0.30	0.35	−2.900 748 507 134 5	1.418 859 663 654 5	0.927 580 543 426 0
0.1	25	25	0.25	0.30	−2.891 910 703 103 4	1.409 741 024 094 0	0.922 195 532 048 2
0.25	25	25	0.25	0.25	−2.833 069 315 397 0	1.359 681 803 628 3	0.892 361 239 021 3
0.5	25	20	0.20	0.20	−2.648 703 149 419 7	1.256 367 735 297 2	0.829 664 522 705 9
1	25	20	0.20	0.20	−2.073 035 362 051 9	1.085 685 768 624 2	0.723 644 141 701 0
2	20	20	0.15	0.15	−0.493 173 861 504 2	0.879 296 076 448 4	0.592 319 993 998 0
5	20	20	0.10	0.10	5.555 021 418 896 5	0.619 377 584 617 5	0.422 804 512 778 6
10	20	20	0.06	0.06	17.162 191 374 057 4	0.459 421 428 281 5	0.316 272 749 895 5

for $N = N_z = 20$. The results are quite insensitive to variations of h_z in this interval. Rounding errors start to slightly deteriorate the accuracy around $N = N_z = 30$. For small values of ω, the convergence is very similar to the free-atom case. See e.g. Table 1 of Ref. [17].

The Lagrange-mesh results for various ω values are presented in Table 2. The values for the free atom ($\omega = 0$) have an accuracy of about 10^{-13} like in Ref. [17]. A relative accuracy of 10^{-12} is already obtained with $N = N_z = 20$. The confinement reduces

Table 3: Convergence of the ground-state energy and the mean interparticle distances of a helium atom confined by potential (52) with $V_0 = 100$ and $R = 4$. The scaling parameters are $h = 0.10$ and $h_z = 0.15$.

N	N_z	N_T	E	$\langle r_{12} \rangle$	$\langle r_1 \rangle = \langle r_2 \rangle$
10	10	950	2.389 517 6	0.717 239 6	0.487 082 6
15	15	1800	2.389 521 083 273	0.717 240 933 789	0.487 083 296 959
20	20	4200	2.389 521 083 370 13	0.717 240 933 821 09	0.487 083 296 966 05
25	25	8125	2.389 521 083 370 11	0.717 240 933 821 11	0.487 083 296 966 08
Ref. [12]			2.389 531		

the size of the atom when ω increases while increasing its energy. The scale factors for the weakest confinement are inspired by those of a free atom. When ω increases, they progressively decrease. To obtain a constant accuracy (thirteen significant digits), the numbers N and N_z can both decrease when the confinement becomes stonger. The present energies confirm the six-digit results of Ref. [12] for $\omega \leq 1$, up to a possible rounding.

Table 4: Ground-state energy and mean interparticle distances of a helium atom confined by potential (52) as a function of the numbers N and N_z of mesh points and the scale parameters h and h_z.

R	N	N_z	h	h_z	E	$\langle r_{12} \rangle$	$\langle r_1 \rangle = \langle r_2 \rangle$
$V_0 = 25$							
1	20	20	0.10	0.10	9.005 664 919 615 0	0.574 015 409 803 2	0.392 137 172 502 8
2	20	20	0.10	0.10	2.205 633 821 802 6	0.732 574 434 299 6	0.496 887 442 688 1
3	20	20	0.10	0.15	0.058 610 162 109 7	0.843 146 864 040 8	0.568 830 018 099 1
4	20	20	0.10	0.15	−0.937 974 874 207 4	0.926 139 670 492 3	0.622 265 713 845 8
5	20	20	0.15	0.15	−1.493 463 026 587 6	0.991 265 922 032 1	0.663 853 999 500 4
10	20	20	0.20	0.30	−2.440 318 186 433 3	1.180 598 995 124 2	0.782 896 512 886 3
25	25	20	0.30	0.35	−2.814 574 813 589 3	1.346 698 806 392 7	0.884 554 240 409 3
100	25	20	0.30	0.35	−2.897 788 906 088 7	1.415 741 535 946 4	0.925 741 063 258 9
$V_0 = 100$							
1	25	25	0.08	0.08	25.983 328 462 164 7	0.407 916 008 582 9	0.281 363 150 279 2
2	20	20	0.10	0.10	9.919 341 323 720 1	0.543 627 679 286 8	0.372 439 834 111 5
3	20	20	0.10	0.10	4.812 589 834 533 1	0.640 875 449 304 4	0.436 905 248 671 5
4	20	20	0.10	0.15	2.389 521 083 370 1	0.717 240 933 821 1	0.487 083 296 966 1
5	20	20	0.10	0.15	1.006 687 798 027 9	0.780 044 762 396 9	0.528 060 835 913 2
10	25	20	0.20	0.25	−1.474 872 423 516 3	0.985 908 228 888 3	0.660 518 629 618 2
25	25	20	0.30	0.35	−2.586 842 706 183 4	1.230 821 212 175 1	0.813 965 678 584 9
100	25	20	0.30	0.35	−2.880 323 145 511 2	1.398 590 911 428 2	0.915 588 071 052 0

As a second potential with a penetrable confinement, we choose like in Ref. [12]

$$V_{\text{conf}}(r_1, r_2) = V_0 \left(2 - e^{-r_1^2/R^2} - e^{-r_2^2/R^2}\right), \tag{52}$$

where V_0 and R are parameters.

The convergence is studied in Table 3 for $V_0 = 100$ and $R = 4$ as a function of N and N_z. Good values of the scale factors are much smaller than for the free atom [17]. Here they are roughly optimized as $h = 0.1$, $h_z = 0.15$. The convergence is very fast. Good results are already obtained with $N = N_z = 10$. An accuracy of about 14 digits is obtained with $N = N_z = 20$ for the energy and for the mean distances.

The Lagrange-mesh energies and mean distances are displayed in Table 4 for $V_0 = 25$ and 100 and some values of R. The scale parameters are rather small for $R = 1$ and must increase with R. The ground-state energy is positive for the smaller R values but the three-body system is nevertheless deeply bound with respect to the asymptotic value $2V_0$ of the confinement potential. Hence the wave functions decrease rather fast. Even for $R = 10$, the properties significantly differ from the free atom. The mean distances are scaled down with respect to the free atom [17] but $\langle r_{12} \rangle$ and $\langle r_1 \rangle$ indicate that the confinement does not change much the shape of the electron distribution. Indeed, the ratio $\langle r_{12} \rangle / \langle r_1 \rangle$ progressively increases from the value 1.45 at strong confinement ($R = 1$, $V_0 = 100$) to the free value 1.53. Our results confirm the four- and six-digit energies of Ref. [12] except for their last two digits displayed at $R = 4$ and 5.

6.2 Hard confinement

Now we consider a nucleus confined in an impenetrable sphere. There are no scale parameters as the size is fixed by the radius R. Otherwise, the code for the new coordinate system follows the same philosophy as the previous one. The total mesh size is $N_T = \frac{1}{2}N(N+1)N_w$ for singlet states and $N_T = \frac{1}{2}N(N-1)N_w$ for triplet states. The mean values are calculated from (50) with (32).

The convergence of Lagrange-mesh results for the ground state is studied in Table 5 for various values of R, as a function of N and N_w. For large R, the convergence is rather slow but it is extremely fast for small R. One obtains 15 significant figures for $R = 0.1$ and 1 but only 11 for $R = 10$. The situation is reversed with respect to soft-confinement calculations in perimetric coordinates where larger bases are needed at small R. The results are compared with Refs. [10, 12, 14, 16]. A good agreement with six significant digits is observed for the most recent results.

Energies and mean distances for the ground state are gathered in Table 6 for a number of R values. The energies confirm the six-digit variational energies of Ref. [12] from 0.5 to 10 and Ref. [16] from 1 to 10. The present coordinate system allows a better description of smaller R values. The earlier variational energies of Ref. [10] have an absolute accuracy below 0.001. This reference is the only one to present $\langle r_{12} \rangle$ mean distances. Their accuracy increases from 10^{-4} to 0.002 when R varies from 0.5 to 6.

Table 5: Convergence of the ground-state energy and the mean interparticle distances of a helium atom confined in a sphere of radius R as a function of the numbers N and N_w of mesh points and the total mesh size N_T.

N	N_w	N_T	E	$\langle r_{12}\rangle$	$\langle r_1\rangle = \langle r_2\rangle$
$R = 0.1$					
8	8	288	906.562 407 9	0.069 580 385 8	0.049 501 241 0
10	10	550	906.562 422 907	0.069 580 382 888 07	0.049 501 246 332 6
10	15	825	906.562 422 919 887	0.069 580 382 884 17	0.049 501 246 340 126
15	15	1800	906.562 429 919 886	0.069 580 382 884 17	0.049 501 246 340 120
15	20	2400	906.562 422 919 888	0.069 580 382 884 16	0.049 501 246 340 121
Ref. [14]			906.562 423		
$R = 1$					
10	10	550	1.015 754 975 53	0.643 664 253 93	0.441 796 632 210
10	15	825	1.015 754 975 90	0.643 664 253 871 0	0.441 796 632 098 55
15	15	1800	1.015 754 976 048 33	0.643 664 253 878 0	0.441 796 632 103 28
15	20	2400	1.015 754 976 048 41	0.643 664 253 877 9	0.441 796 632 103 31
20	20	4200	1.015 754 976 048 64	0.643 664 253 878 0	0.441 796 632 103 34
20	25	5250	1.015 754 976 048 66	0.643 664 253 877 8	0.441 796 632 103 41
25	30	9750	1.015 754 976 048 67	0.643 664 253 878 8	0.441 796 632 103 34
30	35	16275	1.015 754 976 048 54	0.643 664 253 876 9	0.441 796 632 103 24
Ref. [10]			1.015 870	0.643 938	
Refs. [12, 14]			1.015 755		
$R = 10$					
15	15	1800	−2.904 79	1.420 767 962 81	0.928 645 755 91
15	20	2400	−2.903 727 2	1.422 072 790 04	0.929 474 322 57
20	25	5250	−2.903 724 382 6	1.422 070 196 74	0.929 472 263 15
25	30	9750	−2.903 724 375 625	1.422 070 173 66	0.929 472 251 58
30	30	13950	−2.903 724 375 691	1.422 070 172 98	0.929 472 251 22
30	35	16275	−2.903 724 375 668	1.422 070 172 34	0.929 472 250 87
35	35	22050	−2.903 724 375 687	1.422 070 172 96	0.929 472 251 21
Refs. [12, 16]			−2.903 724		

Table 6: Ground-state energy and mean interparticle distances of a helium atom confined in a sphere of radius R as a function of the numbers N and N_w of mesh points.

R	N	N_w	E	$\langle r_{12}\rangle$	$\langle r_1\rangle = \langle r_2\rangle$
0.1	15	15	906.562 422 919 888	0.069 580 382 884 2	0.049 501 246 340 1
0.2	15	20	206.151 712 932 762	0.138 365 789 025 0	0.097 969 984 584 9
0.3	15	20	82.334 517 028 118	0.206 218 777 530	0.145 352 111 929 9
0.4	15	20	40.980 280 331 705 1	0.273 001 759 106	0.191 591 659 047 2
0.5	15	20	22.741 302 819 133 5	0.338 577 477 653	0.236 631 213 255 9
0.6	15	20	13.318 127 241 828 1	0.402 809 660 984	0.280 412 455 464 5
0.7	15	20	7.925 216 046 579 6	0.465 563 856 457	0.322 876 819 396 5
0.8	15	20	4.610 407 554 239 4	0.526 708 460 703	0.363 966 277 267 4
0.9	15	20	2.463 235 988 621 0	0.586 115 943 465	0.403 624 249 990 8
1.0	15	20	1.015 754 976 048 4	0.643 664 253 878	0.441 796 632 103 3
2.0	20	20	−2.604 038 275 176 2	1.097 202 490 172	0.733 956 380 589 2
3.0	25	25	−2.872 494 886 475 7	1.322 925 949 994	0.871 985 220 059
4.0	25	25	−2.900 485 763 363 2	1.399 878 118 648	0.916 962 790 629
5.0	30	30	−2.903 410 849 203 1	1.418 255 199 620	0.927 363 648 349
6.0	30	30	−2.903 695 908 930 7	1.421 528 373 775	0.929 176 980 774
7.0	35	35	−2.903 721 911 531 8	1.422 002 693 115	0.929 435 862 703
8.0	35	35	−2.903 724 170 713 6	1.422 062 567 876	0.929 468 183 475
9.0	35	35	−2.903 724 360 207	1.422 069 437 714	0.929 471 860 371
10.0	35	35	−2.903 724 375 687	1.422 070 172 936	0.929 472 251 212

From the radius dependence of the energies $E(R)$, one can deduce the pressure acting on the confined atom [10, 12, 16],

$$P = -\frac{1}{4\pi R^2}\,\frac{dE}{dR}. \tag{53}$$

The derivative is performed numerically with a 4-point finite-difference formula. The results are presented in Table 7. As before, the significant digits are estimated by comparison between several calculations differing by the number of mesh points. Only those digits are displayed in Table 7. The results are presented both in atomic units and in atmospheres (1 a.u. $= 2.903\,628\,236\,775 \times 10^8$ atm).

A high accuracy is reached up to $R = 2$. Beyond that value, the differences between neighboring energies become tiny and the relative error increases. The results are compared with several earlier variational calculations. The pressures of Ref. [10] have a relative accuracy better than 10^{-4} at $R = 0.5$ and still better than 10^{-3} up to $R = 2$. They become quite poor beyond $R = 4$ as could be expected from the comparison between their variational calculations with different basis sizes. The results of Ref. [12] are consistent with ours for the three displayed digits except at $R = 5$ and 8. The pressures of Ref. [16] have a relative accuracy varying between 0.001 and 0.006.

Energies and mean distances for the first excited singlet level are presented in Table 8. Obtaining the same accuracy as for the ground state sometimes requires

Table 7: Pressure acting on a helium atom confined in a sphere of radius R in a.u. and atm. The powers of ten are indicated between brackets.

R	N	N_w	P (a.u.)	P (atm)	Ref. [10]	Ref. [12]	Ref. [16]
0.1	20	20	1.507 426 738 64[5]	4.377 006 843 19[13]			
0.2	20	20	4.512 880 064 60[3]	1.310 372 598 48[12]			
0.3	20	20	5.682 940 282 5 [2]	1.650 114 587 2 [11]			
0.4	20	20	1.287 118 285 1 [2]	3.737 312 996 8 [10]			
0.5	20	20	4.017 215 609 5 [1]	1.166 450 067 7 [10]	1.166 40[10]	1.167[10]	
0.6	20	20	1.534 428 733 1 [1]	4.455 410 596 9 [9]	4.454 36[9]	4.455[9]	
0.7	20	20	6.732 316 374 6	1.954 814 392 4 [9]	1.954 50[9]	1.954[9]	
0.8	20	20	3.266 880 610 6	9.485 806 787 1 [8]	9.484 10[8]	9.485[8]	
0.9	20	20	1.710 917 738 5	4.967 869 056 3 [8]	4.967 03[8]	4.967[8]	
1.0	20	20	9.510 085 662 1 [-1]	2.761 375 326 3 [8]	2.760 49[8]	2.762[8]	
2.0	25	25	1.383 499 912 [-2]	4.017 169 411 [6]	4.014 56[6]	4.018[6]	4.007 29[6]
3.0	25	25	6.192 831 39 [-4]	1.798 168 01 [5]	1.791 50[5]	1.798[5]	1.793 91[5]
4.0	25	25	3.702 241 59 [-5]	1.074 993 32 [4]	1.086 77[4]	1.074[4]	
5.0	30	30	2.365 111 17 [-6]	6.867 403 58 [2]	9.021 94[2]	6.882[2]	6.850 3 [2]
6.0	30	30	1.526 228 5 [-7]	4.431 600 1 [1]	1.330 15[2]	4.434[2]	
7.0	35	35	9.871 147 [-9]	2.866 214			2.847 95
8.0	35	35	6.399 98 [-10]	1.858 31 [-1]		1.868[-1]	
9.0	35	35	4.161 4 [-11]	1.208 3 [-2]			
10.0	35	35	2.711 [-12]	7.874 [-4]			

higher numbers of mesh points. At $R = 0.1$, the excitation energy exceeds 1000 a.u. For $R = 3$, 5, 7 and 10, a comparison is possible with Ref. [16]. The six-digits results of Ref. [16] agree with the present ones at the level of 10^{-6}. The best variational energies of Ref. [13] have an accuracy around one percent.

Energies and mean distances for the lowest triplet level are gathered in Table 9. They are obtained from the lowest-energy solution for the spatially antisymmetric state. The numbers of mesh points are very close to those for the ground state. At $R = 0.1$, the excitation energy reaches about 1500 a.u. The 2^3S state is thus above the 2^1S contrary to the free-atom situation as already observed in Ref. [13]. This is probably due to the additional constraint that the wave function must vanish for $r_1 = r_2$ in a tiny space. The usual ordering is recovered around $R = 1$ with an excitation energy of about 5 a.u. At all confinements, the triplet state is slightly less extended than the singlet excited state like for the free atom [27]. The best variational energies of Ref. [13] reach an accuracy of abour 10^{-4} above $R = 1$. Below that value the perturbation approach is more accurate; its relative accuracy improves from about 10^{-3} at $R = 1$ to about 10^{-4} at $R = 0.1$.

7 Concluding remarks

Various types of helium confinement can be accurately treated with the Lagrange-mesh method. They are based on the perimetric coordinates for soft confinements or on a new coordinate system for the hard confinement. The method rapidly leads to a large

Table 8: Energy and mean interparticle distances of the 2^1S singlet level of a helium atom confined in a sphere of radius R.

R	N	N_w	E	$\langle r_{12}\rangle$	$\langle r_1\rangle = \langle r_2\rangle$
0.1	15	15	1963.757 922 041 46	0.077 448 989 286 0	0.059 004 994 435 03
0.2	15	20	477.023 366 387 052	0.155 047 268 447 4	0.117 679 576 745 69
0.3	15	20	205.784 321 398 280	0.232 963 503 164 5	0.176 011 387 866 41
0.4	15	20	112.226 705 249 011	0.311 436 535 890	0.233 983 451 406 40
0.5	15	20	69.550 421 013 503	0.390 828 529 869	0.291 568 743 866 7
0.6	15	20	46.705 530 340 508 9	0.471 731 678 057	0.348 716 226 254 7
0.7	15	20	33.131 390 885 993 4	0.555 200 036 019	0.405 310 225 626 3
0.8	15	20	24.447 862 429 155 2	0.643 293 324 656	0.461 031 786 931 6
0.9	15	20	18.574 582 880 828 5	0.740 350 389 720	0.514 775 812 451 3
1.0	15	20	14.413 766 091 552 3	0.853 808 811 249	0.561 631 072 086
2.0	20	25	0.946 588 473 886 9	1.343 903 122 341	0.883 824 224 122
3.0	25	25	−1.114 121 513 742 1	1.866 351 750 214	1.203 075 085 099
4.0	25	25	−1.717 517 590 226 9	2.408 986 509 893	1.498 595 969 032
5.0	30	30	−1.949 761 321 461 5	2.948 630 420 83	1.782 952 066 008
6.0	30	30	−2.050 702 179 185 3	3.435 878 967 14	2.036 478 158 792
7.0	30	30	−2.098 085 074 432 1	3.858 190 026 36	2.254 322 411 040
8.0	30	30	−2.121 511 222 458 8	4.215 842 573 24	2.437 665 074 483
9.0	35	35	−2.133 453 292 480 3	4.510 572 167 17	2.588 081 892 182
10.0	35	35	−2.139 619 886 178 6	4.744 712 449 44	2.707 196 655 205

but sparse symmetric matrix. The eigenvalue problem is not generalized, even with the new coordinate system for which the basis is not orthogonal. This striking property results from the systematic use of the Gauss quadrature associated with the Lagrange basis. This simplifying approximation does not cost accuracy [3, 5].

The present results improve previous works by at least five orders of magnitude for the energies and allow a very accurate calculation of mean interparticle distances. This is obtained with short computer times on a personal computer. The scale parameters given in the present tables allow avoiding a search for their optimal domain of values in future similar calculations. Together with the energies, approximate wave functions are also available. Their high accuracy is confirmed by the high accuracy on the mean values of the coordinates. They are available for other applications.

A serious challenge is the extension of the method to more than three charged particles because a convenient coordinate system, i.e. where the different Coulomb singularities can be regularized, is not available yet.

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Table 9: Energy and mean interparticle distances of the 2^3S triplet level of a helium atom confined in a sphere of radius R.

R	N	N_w	E	$\langle r_{12}\rangle$	$\langle r_1\rangle = \langle r_2\rangle$
0.1	15	15	2370.727 023 303 97	0.074 235 935 806 89	0.049 746 873 483 20
0.2	15	15	568.187 610 564 046	0.148 106 984 196 29	0.098 978 625 497 15
0.3	15	15	241.491 539 024 040	0.221 580 296 180 99	0.147 681 956 058 43
0.4	15	15	129.543 621 160 698	0.294 623 610 981 39	0.195 843 625 489 01
0.5	15	15	78.820 863 703 3835	0.367 205 348 919 4	0.243 450 531 053 3
0.6	15	15	51.856 719 933 0814	0.439 294 711 654 5	0.290 489 790 185 5
0.7	15	15	35.951 107 383 7302	0.510 861 789 094 4	0.336 948 829 834 9
0.8	15	15	25.855 504 026 1363	0.581 877 672 009 0	0.382 815 481 229 5
0.9	15	15	19.089 233 032 7807	0.652 314 569 086 5	0.428 078 079 126 1
1.0	15	15	14.359 714 920 8699	0.722 145 926 846 8	0.472 725 564 359 7
2.0	15	20	0.560 251 233 73470	1.382 427 667 612 2	0.883 572 145 681 4
3.0	20	25	−1.370 510 610 13706	1.965 771 607 822	1.228 588 674 995 6
4.0	20	30	−1.874 611 596 37791	2.474 178 173 270	1.515 265 802 863
5.0	20	30	−2.048 044 093 51074	2.916 562 529 64	1.755 588 974 154
6.0	30	30	−2.117 816 285 16207	3.298 089 015 33	1.957 801 932 623
7.0	30	30	−2.148 564 470 05490	3.619 012 948 88	2.125 320 088 136
8.0	30	30	−2.162 783 826 65888	3.878 261 844 64	2.259 362 209 113
9.0	30	30	−2.169 481 052 37618	4.076 816 120 79	2.361 388 479 41
10.0	30	30	−2.172 627 252 24936	4.219 554 501 84	2.434 424 170 24

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